SOFTWARE VALIDATION TEST PLAN AND TEST REPORT FOR MODULAR THREE-DIMENSIONAL MULTISPECIES TRANSPORT MODEL (MT3DMS) VERSION 4.5

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SOFTWARE VALIDATION TEST PLAN AND TEST REPORT FOR MODULAR THREE DIMENSIONAL MULTISPECIES TRANSPORT MODEL (MT3DMS) VERSION 4.5

MT3DMS Version 4.5 (MT3DMS hereafter) is a general purpose modular three-dimensional transport model that can simulate advection, dispersion, and chemical reactions of dissolved constituents in groundwater systems (Zheng and Wang, 1999). MT3DMS is often used by hydrogeologists to simulate solute transport in groundwater flow systems. MT3DMS does not simulate groundwater flow, hence, it utilizes groundwater flow fields computed by groundwater flow simulators. An approach commonly practiced is to simulate groundwater flow with MODFLOW and simulate solute transport with MT3DMS. MT3DMS and MODFLOW-2000 (Harbaugh, et al., 2000) are included in GMS Version 5.0. In GMS 5.0 the interaction between these two codes is automated and, as a result, no user developed code is required.

MT3DMS solves the three-dimensional advective-dispersive-reactive equation describing solute transport using Eulerian approaches or mixed Eulerian-Lagrangian approaches. Since no single numerical technique is effective for solving all classes of mass transport problems, the combination of these techniques, each having its own strengths and limitations, offers the best approach for accurately solving the range of groundwater problems commonly encountered. The Eulerian approaches included in MT3DMS include the standard finite difference approach for simulating mass transport and a third-order Total Variation Diminishing (TVD) method with a universal flux limiter. Mixed Eulerian-Lagrangian methods included in MT3DMS include the method of characteristics (MOC), the modified method of characteristics (MMOC), and a hybrid method (HMOC) that combines the strength of the MOC for eliminating numerical dispersion with the computational efficiency of the MMOC (Zheng and Wang, 1999).

The chemical reaction models included in MT3DMS are equilibrium-controlled linear or nonlinear sorption and first-order irreversible decay or biodegradation.

MT3DMS will be utilized to simulate the transport of potential highly contaminated groundwater through surrounding areas of the potential high-level waste repository at Yucca Mountain.

1 SCOPE OF THE VALIDATION

This document establishes the Software Validation Test Plan and Test Report for validating the installation and functionality of MT3DMS. The Software Validation Test Plan and Test Report applies to Version 4.5 of MT3DMS. Because all of the features of the software were not tested under the test plan the validation presented here represents a partial validation of the software. Components of the software that were tested reflect those aspects of the code that were relevant to simulating radionuclide transport in the Yucca Mountain region. Additional components of the software may be tested based on future modeling requirements.

Six tests were performed as part of this validation study. The tests are described in detail in Section 6. The first three test problems are taken from the MT3DMS user's manual and the fourth from Domenico and Schwartz, 1990. The first test considers a one-dimensional advection-dispersion transport problem in a uniform flow field. The numerical solution obtained by MT3DMS was compared with an analytical solution for the problem. The second test considers a similar problem geometry, but the transported species is allowed to sorb onto the porous medium; the third test considers transport of a radioactive solute that is undergoing radioactive decay. The fourth test simulates three-dimensional transport in a uniform flow field. A number of numerical schemes for simulating advective transport are present in MT3DMS. In the last two tests, the accuracy of different numerical schemes is compared for a one-dimensional transport problem.

Both MODFLOW-2000 and MT3DMS can be run in stand-alone mode. In this validation test, we invoke MOFLOW-2000 and MT3DMS through GMS (Groundwater Modeling System) Version 5.1, a pre- and post-processor for both codes. GMS Version 5.1 has been validated previously by CNWRA.

2 REFERENCES

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3 ENVIRONMENT

3.1 Software

MT3D (modular three-dimensional transport model) was originally developed in 1990 by Chunmiao Zheng at S.S. Papadopulos & Associates, Inc., and subsequently documented for the Robert S. Kerr Environmental Research Laboratory of the U.S. Environmental Protection Agency. MT3DMS is the second generation of MT3D, offers significantly more capabilities. It was developed in 1998 with funding from the U.S. Army Corps of Engineers Waterways Experiment Station under the Strategic Environmental Research and Development Program (SERDP). A complete description of the software may be found at The Hydrogeology Group at The University of Alabama website <http://hydro.geo.ua.edu/mt3d/>.

This software validation uses Version 4.5 of MT3DMS in the Windows XP environment. However, the code can be used in other Windows operating environments (e.g., Windows 2000) as well as the Linux and UNIX operating environment. The validation uses MODFLOW-2000 to create the groundwater flow fields. The GMS Version 5.1 graphical user interface is used to support the software validation and to provide a link between the MODFLOW-2000 and MT3DMS.

3.2 Hardware

The program can be run on computers running the Windows 2000/XP or Linux/UNIX operating systems. The minimum requirements are a Pentium II, 300 MHz (or equivalent), 128 MB of RAM, 100 MB of disk space, CD-ROM, and a minimum of 800 × 600 screen resolution with high color.

4 PREREQUISITES

Users should be trained to use MT3DMS, as well as MODFLOW-2000. It is also necessary to have some knowledge of hydrogeology, in particular groundwater flow and mass transport in aquifers.

5 ASSUMPTIONS AND CONSTRAINTS

None.

6 TEST CASES

6.1 One-Dimensional Transport in a Uniform Flow Field: Advection and Dispersion

Comparison of calculated concentrations resulting from analytical solutions and numerical solutions provides a method to validate the accuracy of MT3DMS for a one-dimensional transport model. The benchmark one-dimensional transport problem described in Zheng and Wang (1999) includes four transport scenarios that can be used to validate MT3DMS Version 4.5. The first validation test case considers one-dimensional transport with advection and dispersion (Zheng and Wang, 1999, Case 1b). Analytical solutions for this test case are contained in Domenico and Schwartz (1990), Javandel, et al. (1984) and Bear (1979). These solutions were compared to the numerical solution computed using MT3DMS Version 4.5 as part of the validation exercise.

6.1.1 Test Input

A numerical grid was developed consisting of 101 columns, 1 row, and 1 layer with total lengths in the x, y, and z (where z is positive upward) dimensions of 1,010 m, 1 m, and 1 m, respectively. The porosity and hydraulic conductivity of the system were set to 0.25 and 1 m/day respectively. A hydraulic head gradient of approximately 0.06 was imposed across the model by specifying a hydraulic head drop of 60 m between the upstream and downstream ends of the model. MODFLOW-2000 was used to simulate steady-state groundwater flow across the model domain, and the resulting flow fields were used in MT3DMS. The mean groundwater velocity for the model was approximately 0.23 m/day. The groundwater velocity field was used as an input to MT3DMS. The MOC option of the Advection package in MT3DMS Version 4.5 was used with DCEPS=10^{-5}, NPLANE=1, NPL=0, NPH=4, NPMIN=0, NPMAX=8, and a fixed pattern and one vertical place for initial particle placement, the longitudinal dispersivity was set to 10 m, and molecular diffusion was neglected. A constant concentration of 1 mg/l was applied to the upstream end of the model. The grid Peclet number for the model was 1 m. Solute transport over a 2000 day period was simulated in the test.

MATLAB was used to solve the analytical solution with the parameters given by Zheng and Wang (1999) and for values of *x* ranging from 5 to 1,005 m at 10-m intervals. Additional information on this test is contained in CNWRA Scientific Notebook 727E.

6.1.2 Test Procedure

MT3DMS was run using the flow field generated by MODFLOW-2000. The calculated relative concentrations from the numerical solution were extracted from the OUT file produced by MT3DMS and used in MATLAB for comparison to the analytical solution.

6.1.3 Expected Test Results

The criteria established for successful validation of this test case is that the analytical and numerical solution should agree within ± 5 percent. Based upon results provided by Zheng and Wang (1999), the numerical solution should be almost identical to the analytical solution at high and low relative concentration values, while for remaining values the numerical solution will be slightly higher.

6.1.4 Actual Test Results

Figure 1 displays a comparison of the analytical solution (solid lines) and numerical solution (symbols). The analytical and numerical solutions are nearly identical, and the results are as expected. The root mean square error between the numerical solution and the analytical solution was less than 1 percent.

6.2 One-Dimensional Transport in a Uniform Flow Field: Advection, Dispersion, and Sorption

For the second test case, one-dimensional transport with advection, dispersion, and sorption were simulated (Zheng and Wang, 1999, Case 1c) using MT3DMS Version 4.5. The analytical solutions given by Domenico and Schwartz (1990), Javandel, et al. (1984), and Bear (1979), were compared with the numerical solution to support the validation.

6.2.1 Test Input

The steady-state groundwater flow model described in the previous test case was also used for this test case. The computed flow field was once again used as an input to MT3DMS. For the transport model, the longitudinal dispersivity was set at 10 m, molecular diffusion was neglected, and the retardation factor was set to 5. In the advection package, the MMOC option was used with NLSINK=1, NPSINK=4, and a fixed pattern and one vertical plane chosen for initial particle placement. A constant concentration of 1 mg/l was applied to the upstream end of the model. Solute transport over a 2000 day period was simulated in the test.

MATLAB was used to solve the analytical solution with the parameters given by Zheng and Wang (1999) and for values of *x* ranging from 5 to 1,005 m at 10-m intervals. Additional information on this test is contained in CNWRA Scientific Notebook 727E.

6.2.2 Test Procedure

MT3DMS was run using the flow field produced by MODFLOW-2000 as input. The calculated relative concentrations from the numerical solution were extracted from the OUT file produced by MT3DMS and input into MATLAB for comparison to the analytical solution.

6.2.3 Expected Test Results

For successful validation, the analytical and numerical solution should within ± 5 percent. Based upon results provided by Zheng and Wang (1999), the numerical solution should result in slightly higher concentrations than the analytical solution, especially at relative concentrations ranging from 0 to 0.5 m.

6.2.4 Actual Test Results

Figure 2 illustrates a comparison of calculated concentration with the analytical solution (solid lines) and numerical solution (symbols). The root mean square error between the numerical solution and the analytical solution was approximately 3 percent.

6.3 One-Dimensional Transport in a Uniform Flow Field: Advection, Dispersion, Sorption, and Decay

For the third test case, one-dimensional transport with advection, dispersion, sorption, and decay was simulated using MT3DMS Version 4.5. The analytical solutions given by Domenico and Schwartz (1990), Javandel, et al. (1984), and Bear (1979) were compared with the numerical solution to support the validation.

6.3.1 Test Input

The one-dimensional steady-state groundwater flow model used in the previous examples was used to provide the flow field needed by MT3DMS to support this test. For the transport simulation, the longitudinal dispersivity was set to 10 m, molecular diffusion was neglected, the retardation factor was set to 5, and the decay rate constant (λ) was set to 0.002 d^{-1}. The MMOC option was used to solve the solution with NLSINK=1, NPSINK=5, and a fixed pattern and one vertical plane for initial particle placement. Solute transport over a 2000 day period was simulated in the test.

MATLAB was used to solve the analytical solution with the parameters given by Zheng and Wang (1999) and for values of *x* ranging from 5 to 1,005 m at 10-m intervals. Additional information on this test is contained in CNWRA Scientific Notebook 727E.

6.3.2 Test Procedure

MT3DMS was run using the flow field produced by MODFLOW-2000 as input. The calculated relative concentrations from the numerical solution were extracted from the OUT file produced by MT3DMS and input into MATLAB for comparison to the analytical solution.

6.3.3 Expected Test Results

It is expected that the analytical and numerical solution should agree within ± 5 percent. Based upon results provided by Zheng and Wang (1999), the numerical solution should result in slightly lower concentration than the analytical solution.

6.3.4 Actual Test Results

Figure 3 displays the comparison of the numerical solution (symbols) to the analytical solution (solid line). The root mean square error between the numerical solution and the analytical solution was less than 2 percent.

6.4 Three-Dimensional Transport in a Uniform Flow Field

As in the one-dimensional transport test case, comparison of the calculated concentrations of the analytical and numerical solutions provides a method of validating the accuracy of MT3DMS for three-dimensional transport. The example that served as a test case was provided by Domenico and Schwartz (1990), however, the test case did not include decay. The analytical solution for multidimensional transport with continuous sources supplied by Domenico and Schwartz (1990) was compared with the results from the numerical model.

6.4.1 Test Input

The model domain was 700 × 105 × 50 m in the x, y, and z directions respectively. Note that positive z is upward. The grid spacing in the x-direction was $\Delta x = 1$ m. The grid spacing in the y and z directions were varied during the analysis. A uniform hydraulic gradient of 0.026 in the x-direction was created by applying a 18 m head drop between the model boundaries perpendicular to the x-axis. No-flow conditions were applied across the remaining faces of the model domain. The porosity and hydraulic conductivity of the model were set to 0.3 and 1 m/day, respectively. Steady-state groundwater flow in the model domain was simulated using MODFLOW-2000. The mean groundwater flow velocity in the domain was determined to be approximately 0.09 m/day. The computed steady-state groundwater flow field was used as an input to MT3DMS. The solute transport problem considered a patch source 15 × 10 m placed on the upstream boundary of the model. The patch was further assumed to have a constant concentration of 1 mg/l. For the MT3DMS simulations, the patch was subdivided into 4 (corresponding to approximate grid discretizations of $\Delta y = 7.4$ m and $\Delta z = 5$ m), 9 (corresponding to approximate grid discretizations of $\Delta y = 5$ m and $\Delta z = 3.3$ m), and 16 (corresponding to approximate grid discretizations of $\Delta y = 3.9$ m and $\Delta z = 2.5$ m) cells. The longitudinal, horizontal transverse, and vertical transverse dispersivities were set to 1, 0.1, and 0.01 m, respectively. Molecular diffusion, decay, and sorption were not included in the model. Solute transport over a time period of 5475 days was simulated using both the numerical model and an analytical solution contained in Domenico and Schwartz (1990). Additional information on this test is contained in CNWRA Scientific Notebook 727E.

6.4.2 Test Procedure

MT3DMS was run using the flow field produced by MODFLOW-2000 as input. The calculated relative concentrations from the numerical solution was extracted from the OUT file produced by MT3DMS and input into MATLAB for comparison to the analytical solution.

6.4.3 Expected Test Results

For successful validation, the analytical and numerical solutions should match within ± 5 percent and that as the grid becomes finer, the results of the numerical solution should more closely match the analytical solution.

6.4.4 Actual Test Results

Figure 4 compares the output from the numerical model and the analytical solution. In particular, the figure compares the concentration profile along the centerline of the plumes. As anticipated, the more sources present within the 15 by 10 m zone, the more accurate the numerical solution. For example, when the patch is subdivided into 16 source regions, the root mean square error between the concentration profiles for the analytical and numerical solutions is less than 1 percent. The root mean square error between the two solutions increased to approximately 5 percent when the patch source was subdivided into 4 sources.

6.5 Solution Scheme Comparisons: Advection Dominated Case

Comparison of solution schemes in the Advection package of MT3DMS with an analytical solution provides an approach to evaluate their relative performance for various classes of transport problems. For this test case, a purely advective one-dimensional transport was simulated in order to assess the relative performance of the various solution schemes for this type of problem. It is important to note that advective transport represents one of the more computationally intensive problems in computational hydrology. The analytical solutions given by Domenico and Schwartz (1990) will serve as the basis for comparison.

6.5.1 Test Input

The one dimensional groundwater flow model previously described was used to support this test. For the transport simulation, the longitudinal dispersivities was set to zero. Molecular diffusion, decay, and retardation were all neglected in the simulation. First the method of characteristics (MOC) option was used in the advection package solution with DCEPS=10^{-5}, NPLANE=1, NPL=0, NPH=4, NPMIN=0, and NPMAX=8, followed by the third order TVD scheme (ULTIMATE) and the standard finite difference model with upstream weighting. A constant concentration of 1 mg/l was assigned to the upstream end of the model.

MATLAB was used to solve the analytical solution with the parameters given by Zheng and Wang (1999) and for values of *x* ranging from 5 to 1,005 m at 10-m intervals. Additional information on this test is contained in CNWRA Scientific Notebook 727E.

6.5.2 Test Procedure

MT3DMS was run using the flow field produced by MODFLOW-2000 as input. The calculated relative concentrations from the numerical solutions were extracted from the OUT file produced by MT3DMS and input into MATLAB for comparison to the analytical solution.

6.5.3 Expected Test Results

This analysis was designed to illustrate the relative performance of the various transport schemes for a system in which transport is dominated by advection. It is expected that for this type of problem that the MOC scheme would yield the best solution and the finite difference scheme would yield the poorest solution.

6.5.4 Actual Test Results

Figure 5 displays a comparison of the three solution schemes mentioned above and the analytical solution. As expected, the error between the solution based on the MOC and the analytical solution were within 5 percent of the analytical solution (see CNWRA Scientific Notebook 735). The RMS error associated with the Ultimate scheme was 6 percent (see CNWRA Scientific Notebook 735). The upstream standard finite difference model provides a noticeably poorer representation of the analytical solution. The RMS error associated with this solution was on the order of 10 percent (see CNWRA Scientific Notebook 735). From these results, it can be concluded that the MOC solution scheme is the most accurate scheme to use in a purely advective case. Note that the accuracy of the Ultimate and the finite difference schemes can be improved by reducing the grid spacing.

6.6 Solution Scheme Comparisons: Non-Advection Dominated Case

Comparison of solution schemes in the advection package with the analytical solution provides a way to determine the most accurate solution scheme. For this test case, a one-dimensional transport with advection and dispersion will be simulated in order to determine the most appropriate solutions scheme for this type of problem. The analytical solutions given by Javandel, et. al (1984) will serve as the basis for comparison.

6.6.1 Test Input

The one dimensional groundwater flow model previously described was used to support this test. For the transport simulation, the longitudinal dispersivities was set to 10 m. Molecular diffusion, decay, and retardation were all neglected in the simulation. A constant concentration of 1 mg/l was assigned to the upstream end of the model. First the MOC option was used in the advection package solution with DCEPS=10^{-5}, NPLANE=1, NPL=0, NPH=4, NPMIN=0, and NPMAX=8, followed by the ULTIMATE scheme and the standard finite difference model with upstream weighting, both with one as the maximum number of cells any particle was allowed to move per transport step.

MATLAB was used to solve the analytical solution with the parameters given by Zheng and Wang (1999) and for *x* values ranging from 5 to 1,005 m at 10-m intervals. Additional information on this test is contained in CNWRA Scientific Notebook 727E.

6.6.2 Test Procedure

MT3DMS was run using the MODFLOW-2000 file for each solution scheme, as described above. The calculated relative concentrations from the numerical solutions were extracted from the OUT file produced by MT3DMS and input into MATLAB for comparison to the analytical solution.

6.6.3 Expected Test Results

For successful validation, all solution scheme should be within ± 5 percent of the analytical solution. The finite standard difference model is expected to be slightly less accurate than the MOC and ULTIMATE schemes.

6.6.4 Actual Test Results

Figure 6 shows a comparison of the analytical solution and the three solution schemes for one-dimensional transport with advection and dispersion. All results are within 5 percent root mean square error of analytical results (see CNWRA Scientific Notebook 735). The MOC and ULTIMATE solutions are more accurate than the standard finite difference model. However the standard finite difference model with upstream weighting is more accurate in the case of a non-advection dominated model than a purely advective case. From these results, it can be concluded that any of the solution schemes are acceptable for use in a non-advection dominated transport simulation, however the MOC is the most accurate. Additional investigations and conclusions regarding advection solution schemes are given by Prommer, et. al (2002).

7 INDUSTRY EXPERIENCE

Both MODFLOW and MT3DMS are widely adopted in the environmental consulting industry and have become the de-facto standards for environmental litigation support. Several commercial pre- and post-processors have been developed for the two codes. Numerous numerical studies in the literature were carried out using the two codes. Both codes have evolved significantly in the last two decades since they first became available to the hydrogeology community and thus, they should be considered mature.

8 NOTES

None.

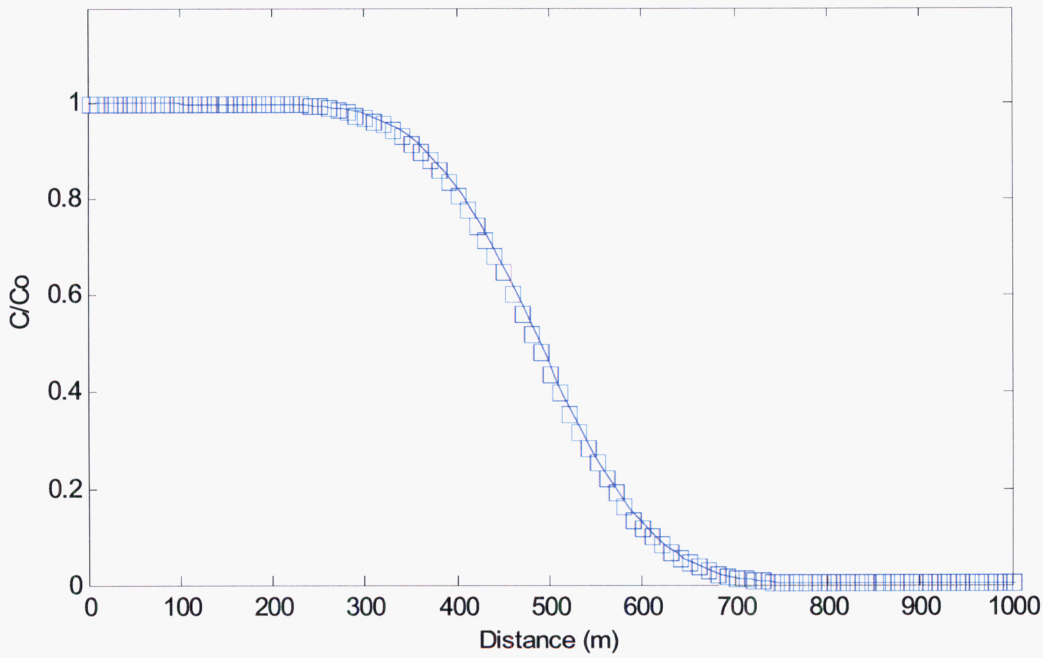

Figure 1. Comparison of the Analytical Solution (Solid Line) and Numerical Solution (Solid) for One-Dimensional Transport with Advection and Longitudinal Dispersion

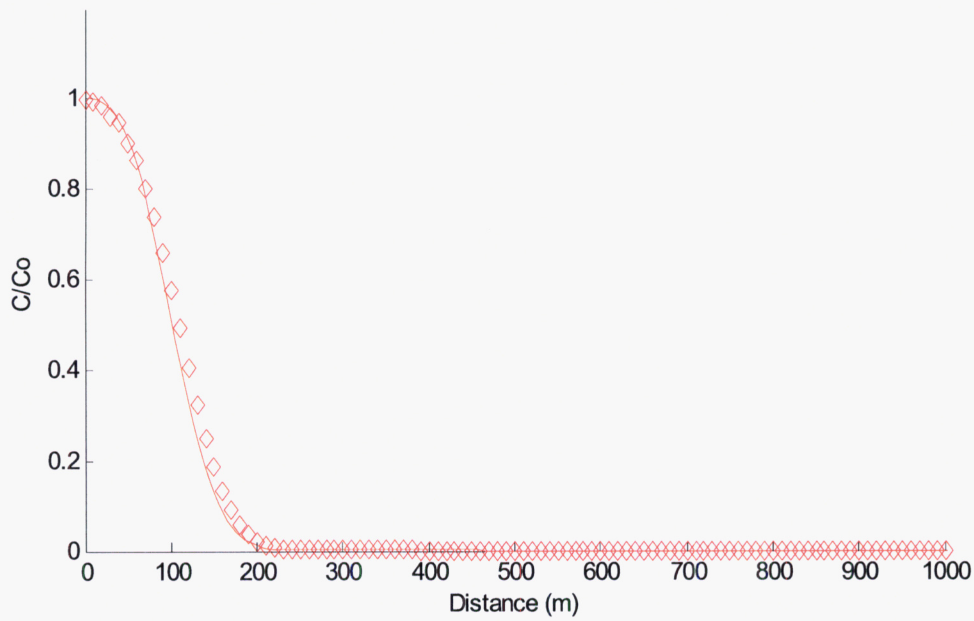

Figure 2. Comparison of the Analytical Solution (Solid Line) and Numerical Solution (Symbols) for One-Dimensional Transport with Advection, Longitudinal Dispersion, and Sorption

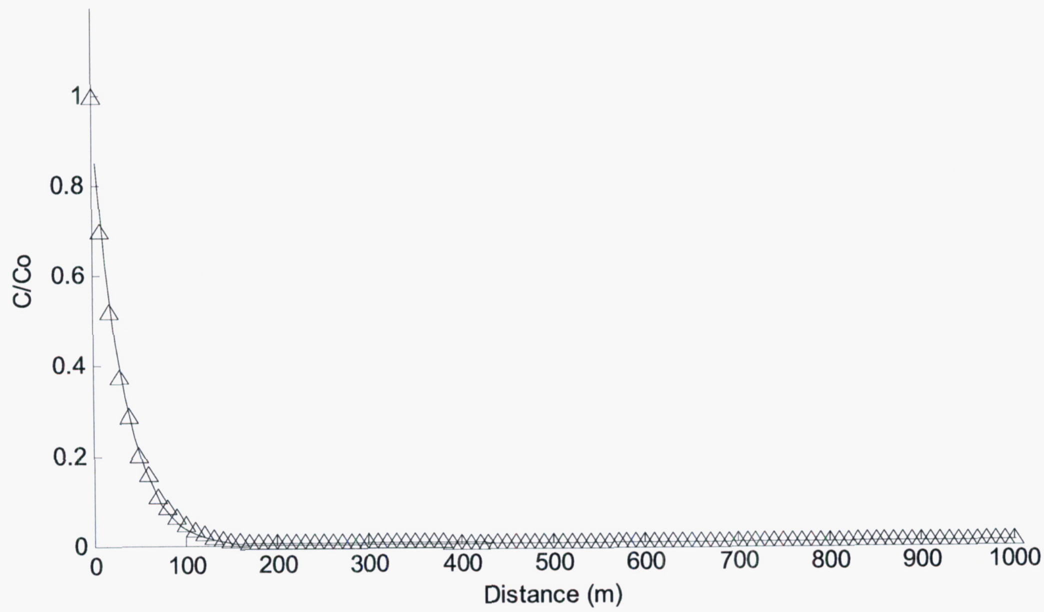

Figure 3. Comparison of the Analytical Solution (Solid Line) and Numerical Solution (Symbols) for One-Dimensional Transport with Advection, Longitudinal Dispersion, Sorption, and Decay

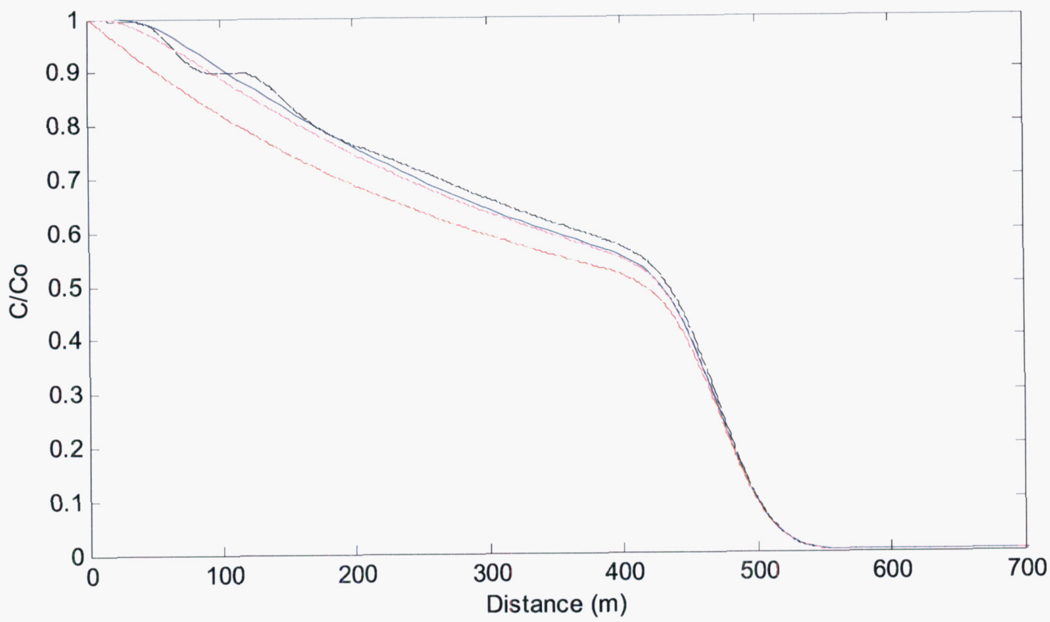

Figure 4. Comparison of the Analytical Solution (Blue) and Numerical Solution with Four (Red), Nine Black), and Sixteen (Magenta) Sources for Three-Dimensional Transport

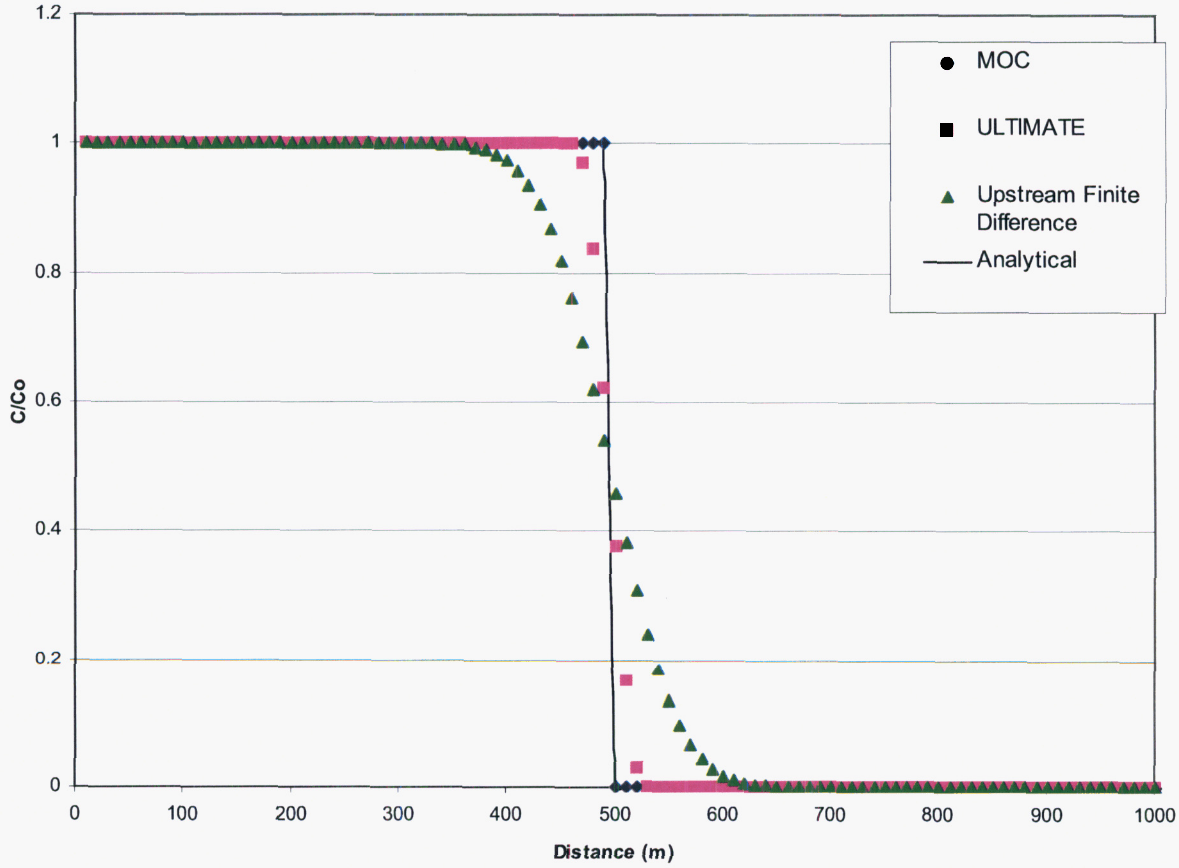

Figure 5. Comparison of the Analytical Solution and Numerical Solutions with Differing Solution Schemes for One-Dimensional Transport with Advection Only

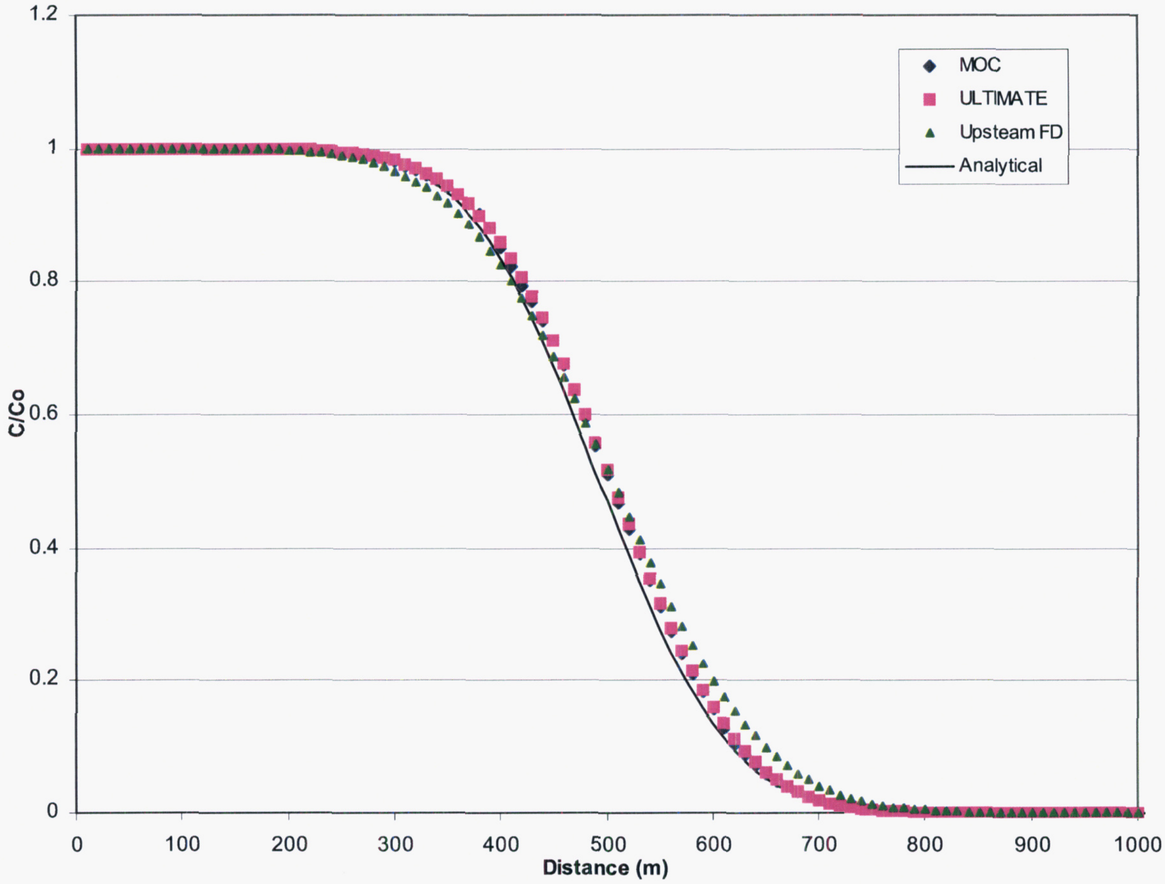

Figure 6. Comparison of the Analytical Solution and Numerical Solutions with Differing Solution Schemes for One-Dimensional Transport with Advection Only